

Dynamics of Many-Body Localization

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Following the field theoretic approach of Basko *et al.*, Ann. Phys. **321**, 1126 (2006), we study in detail the real-time dynamics of a system expected to exhibit many-body localization. In particular, for time scales inaccessible to exact methods, we demonstrate that within the second-Born approximation that the temporal decay of the density-density correlation function is non-exponential and is consistent with a finite value for $t \rightarrow \infty$, as expected in a non-ergodic state. This behavior persists over a wide range of disorder and interaction strengths. We discuss the implications of our findings with respect to dynamical phase boundaries based both on exact diagonalization studies and as well as those established by the methods of Ref. 1.

It has been known for more than 50 years that *non-interacting* particles in a one-dimensional disordered system exhibit Anderson localization [2], namely the exponential suppression of transport. While a localized system is non-ergodic and thus does not thermalize, coupling the system to other degrees of freedom with a continuous spectrum, such as a heat bath, allows thermalization to occur via processes such as variable-range hopping [3]. For an isolated many-body system, only interactions between the particles may lead to thermalization. The question of whether or not localization is stable in the presence of interactions was first considered by Fleishman and Anderson [4], who concluded that short-ranged interactions cannot destabilize the insulating phase. A similar and still open question also exists for Bose-Einstein condensates, treated in the framework of the time-dependent Gross-Pitaevskii (or nonlinear Schrödinger) equation [5]. In this case numerics, as well as analytical arguments, suggest a temporally sub-diffusive or even logarithmic thermalization behavior for not very strong interactions [5].

Using a diagrammatic approach, Basko *et al.* argued that for a general class of isolated, disordered and interacting systems, a many-body mobility edge exists, similarly to the Anderson mobility edge in a three-dimensional non-interacting system [1]. Namely, a critical energy separates “insulating” and “metallic” eigenstates, which can be distinguished by evaluating the spatial correlations of any local operator. “Metallic” eigenstates will have non-vanishing or slowly decaying correlations, while “insulating” states will have exponentially decaying correlations. By changing the energy (or the micro canonical temperature) of the system across the mobility edge, the system will undergo an insulator–metal transition. Similar to the Anderson transition, the many-body localization (MBL) transition is a dynamical and *not* a thermodynamic phenomena [1]. However, the MBL transition is also not a conventional quantum phase transition since the critical energy, which depends on the parameters of the system, may be very far from the ground state. In fact, for systems of bounded energy density (e.g., finite number of states per site), Oganesyan and

Huse suggested that the transition will persist up to infinite temperature [6]. Namely, nontrivial parameters of the system may be found such that essentially *all* the eigenstates are “insulating”. For a zero dimensional system mapped to the Bethe lattice, it was theoretically proposed [7] and recently numerically examined [8], that for some range of parameters the metallic phase can be *non-ergodic*. The existence of a non-ergodic *metallic* phase for *finite* dimensional systems had been conjectured [9], but has been numerically tested only for small systems [10].

By calculation of the DC conductivity or the properties of eigenfunctions for sufficiently small systems, the MBL transition has gained support from numerical studies that utilize either direct diagonalization [6, 11–14] or methods of similar numerical complexity [15]. However, all of these studies suffer from the drawback that the numerically accessible system size is about 16 sites, which does not allow for a systematic analysis of finite size effects. This is not an issue deep within the insulating phase, but due to the divergence of the interacting localization length at the transition, it introduces severe difficulties for examining the system near the putative transition and in the metallic phase. Other studies have examined the dynamical nature of the transition using time-dependent density matrix renormalization group (tDMRG) or similar methods [16, 17]. However, these studies are restricted to the localized phase due to the growth of entanglement entropy. While the existence of an insulating phase for some range of parameters and energies appears to be quite well established even at the rigorous level [18], this is not the case for the metallic phase, where there are currently no rigorous results and the existing numerical schemes are quite limited.

In this letter, we examine the dynamics of an isolated one-dimensional system across the putative MBL transition predicted by exact diagonalization studies of the same system. In particular, we study the relaxation dynamics of our system starting from a far-from-equilibrium initial condition that is a pure state of the corresponding non-interacting system. We follow the diagrammatic approach of Ref. 1, while relaxing several assumptions used

in that work. Unlike the work of Ref. 1, we compute in detail the dynamics of the system from an appropriately chosen initial condition. By doing so, we are able to assess the accuracy of the approximations used in Ref. 1 against exact numerical results (where available) as well as to describe how the MBL transition should manifest within the very framework that first predicted its existence.

Following previous studies [11–16], we investigate a one-dimensional system of spinless and interacting fermions in a disordered potential,

$$H = -t \sum_i \left(\hat{c}_i^\dagger \hat{c}_{i+1} + \hat{c}_{i+1}^\dagger \hat{c}_i \right) + V \sum_i \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_{i+1} - \frac{1}{2} \right) + \sum_i h_i \left(\hat{n}_i - \frac{1}{2} \right), \quad (1)$$

where t is the hopping matrix element, V is the interaction strength and h_i are random fields independently distributed on the interval $h_i \in [-W, W]$. Note that by using the Jordan-Wigner transformation, this model can be exactly mapped onto the XXZ model. There are only two independent parameters in the Hamiltonian and we therefore choose $t = 1$. Since this model has a bounded energy density $|\langle H \rangle|/L \leq (2t + V/4 + W/2)$ (where L is the length of the system), critical parameters may be found such that the system will transition from a mixture of “insulating” and “metallic” states to a situation where *all* of the many-body eigenstates are “insulating.” The existence of such parameters is equivalent to the assumption used in Ref. 6 that the MBL transition will survive at infinite temperature. Under these conditions, the critical disorder strength has been determined in previous studies for rather strong interaction $V = 2t$, to be about $W_c/t \approx 7 - 8$ [12, 13]. Since our approach is based on many-body perturbation theory, we are limited to small interaction strengths. Therefore, to find the relevant critical parameters, we extend the calculations of Ref. 12 to evaluate the critical *line* in the space of W/t and V/t using exact diagonalization (see Fig. 1). We also estimate the theoretical dynamical phase boundaries by using the critical temperatures and a thermodynamic relation [1, 19]

$$T_{el} = \frac{t^2}{\nu \xi V^2}, \quad T_c = \frac{t}{12\nu \xi V \ln t/V}, \quad \frac{E}{L} = \frac{\pi^2}{6} \nu T^2. \quad (2)$$

Here ξ is the non-interacting localization length, T_{el} is the temperature which separates ergodic and non-ergodic metals (see e.g., [9]), T_c is the transition temperature and ν is one-particle density of states. Although for high temperatures and for a system with a bounded energy density the thermodynamic relation is not strictly valid, we use it to extrapolate from low to high temperatures by setting E_c/L to be equal to half of the energy band

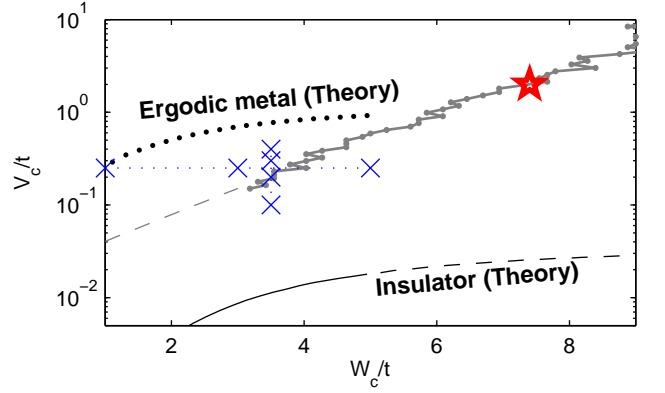


Figure 1: (color online) Dynamical phase boundaries of the system as a function of W/t and V/t . Gray solid line indicates the numerical critical values calculated using the method of Ref. 12 ($N = 12$, see their Fig. 6). The red star represents the transition point obtained in Ref. 12 (note the factor of 2 difference in W_c). The blue crosses represent the parameters used in this work. Vertical cut: $W = 3.5$ and $V = 0.1, 0.2, 0.3, 0.4$. Horizontal cut: $W = 1, 3, 5$ and $V = 0.25$. The solid black line is the solution of Eq. (3), and separates metal from insulator. The dotted black line is obtained from Eq. (2), and demarcates the boundary between ergodic and non-ergodic metals. The dashed lines are extrapolations to regions below which such equations are *not* valid.

$\Delta \approx (2t + W/2)$ (the interaction contribution is negligible) [19]. The critical interaction can now be obtained in terms of the non-interacting localization length, $\xi(W)$ and W ,

$$\frac{V_{el}}{t} = \frac{1}{\sqrt{\alpha}}, \quad \frac{V_c}{t} = \frac{1}{12\alpha (\ln 12\alpha (\ln (12\alpha \dots)))}, \quad (3)$$

where $\alpha = \sqrt{6\nu \Delta \xi^2 / (\pi^2 t)}$. The theoretical lines are valid for $V_c/t < 1$ and $\xi > 1$, and are plotted at Fig. 1. It is clearly seen that the numerical critical line is one order of magnitude higher than the theoretical one, lying predominately in the non-ergodic metal phase. We will show, however, that at least for small interaction strengths the numerical critical line suffers from severe finite size effects. Taking this into account suggests that the line should move towards higher values of V , which will drive it even further away from the phase boundary where theory predicts a stable insulator. One possible explanation of this discrepancy could be that the insulating phase is stable up to T_{el} and not T_c as predicted by the theory. In other words, the non-ergodic metal phase is also insulating. Alternatively, the approach used to determine the numerical critical line [12] might be sensitive to an ergodic non-ergodic transition within the metal phase and not the true metal-insulator transition.

We next outline our dynamic scheme which is similar in spirit to Ref. 1, but relaxes several approximations of that work. We start with the one-particle greater and

lesser non-equilibrium Green's functions,

$$\begin{aligned} G_{ij}^>(t; t') &= -i\text{Tr} \left\{ \hat{\rho}_0 \hat{c}_i(t) \hat{c}_j^\dagger(t') \right\} \\ G_{ij}^<(t; t') &= i\text{Tr} \left\{ \hat{\rho}_0 \hat{c}_j^\dagger(t') \hat{c}_i(t) \right\}, \end{aligned} \quad (4)$$

where $\hat{\rho}_0$ is the initial density matrix. For a non-interacting initial density matrix, the Green's functions obey the Kadanoff-Baym equations of motion [20],

$$\begin{aligned} i\partial_t G^\gtrless(t, t') &= \left(\hat{h}_0 + \Sigma^{HF}(t) \right) G^\gtrless(t, t') \\ &+ \int_0^t \Sigma^R(t, t_2) G^\gtrless(t_2, t') dt_2 \\ &+ \int_0^{t'} \Sigma^\gtrless(t, t_2) G^A(t_2, t') dt_2, \end{aligned} \quad (5)$$

where spatial indices and summations are suppressed for clarity; $\hat{h}_{0,nm} = -t(\delta_{n,m+1} + \delta_{n,m-1}) + h_n \delta_{nm}$ is the one particle Hamiltonian; $\Sigma^{HF}(t)$, $\Sigma^\gtrless(t)$ are the Hartree-Fock greater and lesser self-energies of the problem respectively; and the superscripts 'R' and 'A' represent retarded and advanced Green's functions and self-energies, which are defined as

$$\begin{aligned} \Sigma^R(t, t_2) &= \theta(t - t_2) (\Sigma^>(t, t_2) - \Sigma^<(t, t_2)) \\ G^A(t_2, t') &= -\theta(t' - t_2) (G^>(t_2, t') - G^<(t_2, t')). \end{aligned} \quad (6)$$

Note that due to the complexity of (5), what was actually considered in Ref. 1 is the corresponding quantum Boltzmann equation. For this purpose the authors have neglected the off-diagonal spatial elements of the Green's functions, and performed a gradient expansion of the time variable. Additionally, the real part of the self-energy as well as the Hartree-Fock contributions have been neglected [1]. Although it is numerically feasible to solve (5) within the specified approximation for the self-energies (see below), this approach turns unstable for sufficiently long times of any parameters of the Hamiltonian. To eliminate this spurious behavior we reduce (5) to a quantum master equation for the one-particle density matrix by introduction of the generalized Kadanoff-Baym ansatz,

$$G^\gtrless(t, t') = i \left[G^R(t, t') G^\gtrless(t', t') - G^\gtrless(t, t) G^A(t, t') \right], \quad (7)$$

and by approximating the retarded and advanced Green's functions with their Hartree-Fock (HF) values [21–23]. This approach is in the spirit of the Boltzmann approach of Ref. 1, and is ostensibly more precise, since it considers the full density matrix and not just its diagonal values. Additionally, the quasi-classical approximation as well as gradient expansions are not needed, which allows us to describe systems far from equilibrium. It is not our purpose to examine the validity of this approximation in this letter and the reader is referred to Refs. 21, 22. We leave

the discussion of the full solution of (5) to a future study. As in Ref. 1 we utilize both the HF and the self-consistent second-Born (2B, called SCBA in [1]) approximations for the self energies,

$$\begin{aligned} \Sigma_{ij}^{HF}(t) &= -i\delta_{ij} \sum_k V_{ik} G_{kk}^<(t; t) + iV_{ij} G_{ij}^<(t; t) \\ \Sigma_{ij}^>(t, t') &= \sum_{k,l} V_{il} V_{jk} G_{kl}^<(t', t) \times \\ &\quad \left[G_{lk}^>(t, t') G_{ij}^>(t, t') - G_{lj}^>(t, t') G_{ik}^>(t, t') \right], \end{aligned} \quad (8)$$

where $V_{ij} = V(\delta_{i,j+1} + \delta_{i,j-1})$ is the interaction potential.

The fact that the insulating phase is non-ergodic means that great care must be exercised with regards to the choice of the initial conditions [1, 19]. To illustrate the issues involved, consider a disconnected interacting system, namely by setting $t = 0$. This system can be solved exactly, given the fact that the Hamiltonian is already diagonal in the position basis. A similar model was studied by several authors in the context of the MBL, but for distinct purposes, see Refs. 24, 25. The Green's function is a periodic function of time with period V . Ignoring the fact that the system is solvable and utilizing the diagrammatic perturbation theory up to second order in V (as in the 2B approximation) gives,

$$\Sigma_i^<(t) = i \langle \hat{n}_i \rangle e^{-i\epsilon t} \sum_j V_{i,j} \langle \hat{n}_j \rangle \langle 1 - \hat{n}_j \rangle, \quad (9)$$

where $\langle \hat{n}_j \rangle = \text{Tr} \hat{\rho}_0 \hat{n}_j$. Notably, the imaginary part of the self-energy yields an unphysical decay of the Green's function, and only vanishes if $\langle \hat{n}_i \rangle = n_i = 0, 1$ (which implies a density matrix which is one Slater determinant localized on lattice sites). It can be shown that with this form of initial density matrix the problem may be solved using only the Hartree term. Thus, if we would like to recover the proper $t \rightarrow 0$ limit in the framework of 2B, any selected initial state should have the properties disclosed above in this limit. To satisfy this restriction, we use the following initial condition:

$$G_{ij}^<(0, 0) = i \sum_k \phi_k(i) \phi_k(j) n_k^0, \quad (10)$$

where $n_k^0 \in (0, 1)$, and $\phi_k(i)$ are the non-interacting one-particle eigenstates. We consider half-filling throughout this letter, although other fillings have been investigated and do not lead to distinct behavior.

For a MBL transition at finite temperature, the mobility edge is found within the many-body spectrum, and therefore the average energy as well as the energetic width of the initial condition are of great importance, since they determine the position of the state with respect to the many-body mobility edge. For a MBL transition at infinite temperature, for certain parameters, *all*

eigenstates become “insulating,” and therefore the initial condition should not be important. Nevertheless, to eliminate one control parameter, we set the location of the mean energy density of the initial condition to be in the middle of the many-body energy band, namely $\langle H \rangle = 0$. This closely corresponds to the $T \rightarrow \infty$ limit invoked in Ref. 6, and allows one to establish the onset of the transition when the mobility edge converges to zero. The relaxation of the system is monitored by calculating the correlation function

$$\delta\rho(t) = \frac{1}{L} \sum_k \overline{\left\langle \left(\hat{n}_k(t) - \frac{1}{2} \right) \left(\hat{n}_k(0) - \frac{1}{2} \right) \right\rangle}, \quad (11)$$

where $\hat{n}_k = \sum_{ij} \phi_k(i) \phi_k(j) \hat{c}_i^\dagger \hat{c}_j$, and the over-line indicates averaging over disorder realizations. Generically a two-particle Green’s function is needed to calculate this quantity, however the chosen initial condition (10) renders $\langle \hat{n}_k(t) \hat{n}_k(0) \rangle = \langle \hat{n}_k(t) \rangle \langle \hat{n}_k(0) \rangle$. Since the total number of particles is conserved, this correlation function measures the diffusion rate of the one-particle energy, and for an initial conditions in the ergodic phase it will typically decay as $t^{-1/2}$ or faster as a function of time (see, e.g., Ref. 26 for studies of clean systems). For initial conditions in a non-ergodic phase temporal decay will cease after some finite time, or alternatively, a subdiffusive relaxation is expected. Note that although a non-decaying correlation indicates that some of the particles are pinned to their initial positions, it does not preclude a finite mobility for the rest of the particles, and therefore does not rule out metallic behavior. Nevertheless, in this case the mobility of the particles is expected to be considerably impaired with comparison to the ergodic case. It is precisely this non-ergodic conducting situation which defines the non-ergodic metal region of the dynamic phase diagram of Fig. 1.

We solve the quantum master equation (QME) numerically for the one-particle Green’s functions (5) as a function of time, with the initial conditions (10) and the self-energies (8). For this purpose we use the numerical method developed in [27]. The correlation function is averaged over 256 realizations of the disordered potential. In Fig. 2a we compare the perturbative calculation to the exact solution of a small chain, $L = 12$, obtained by exact diagonalization (ED). A remarkable correspondence between the QME and the exact solutions is seen for $V = 0.25$ and times $t \lesssim 40$. This correspondence becomes better for larger W and does not exist at the HF level, which produces only non-decaying solutions (not shown). For longer times there is only a qualitative correspondence between the QME and the exact solution. It should also be noted that for smaller values of W such as $W = 1$ (where the non-interacting localization length, $\xi = 25$, is larger than the system size) the $L = 12$ system is simply a model for testing the approximation scheme and has little bearing on the dynamics of MBL in the

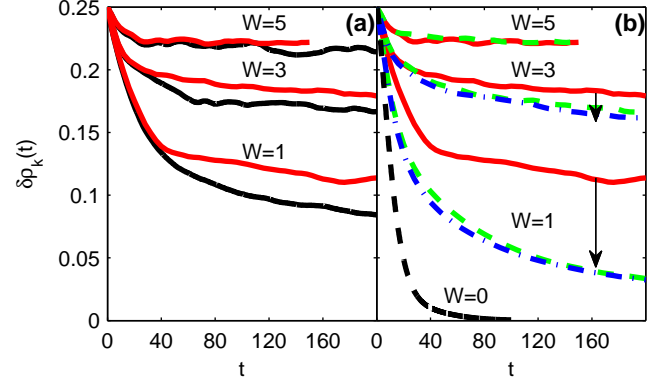


Figure 2: (color online) **(a)** Density-density correlation function as a function of time for averaged over 256 disorder realizations ($V = 0.25$). The solid black lines designate the exact solution calculated using ED ($L = 12$) and red (gray) lines designate the solution using QME. **(b)** Finite size behavior for same parameters using QME. The system sizes used: $W = 0$, $N = 2^{14}$ (black dashed); $W = 1$, $N = 12, 48, 96$ (solid, dashed, dot dashed); $W = 3$, $N = 12, 28, 36$ (solid, dashed, dot dashed) and $W = 5$, $N = 12, 28$ (solid, dashed).

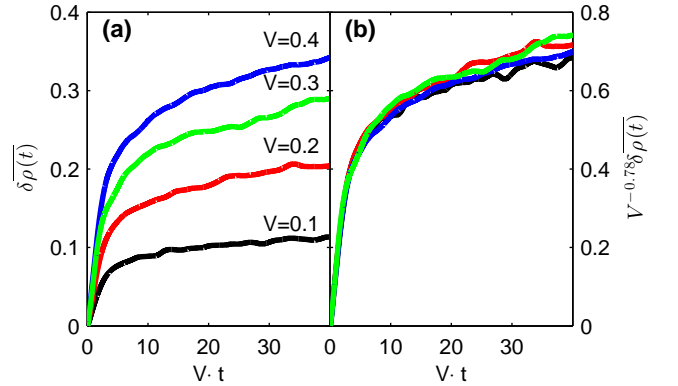


Figure 3: (color online) **(a)** Modified density-density correlation ($\delta\bar{\rho}(t) \equiv 1 - 4\delta\rho(t)$) as a function of $V \cdot t$, averaged over 256 disorder realizations, for $W = 3.5$, $L = 36$. **(b)** Left panel rescaled by plotting $V^{-0.78} \delta\bar{\rho}$ as a function of $V \cdot t$ (see text).

thermodynamic limit, although surprisingly the dynamics is not very different from that at much larger disorder strengths.

From Fig. 2b we observe that after the initial relaxation there is a slow decay of the correlation function. The decay of the clean system is exponential with a time scale of $t_1 \sim V^{-2}$, which indicates that the QME within the 2B approximation *overestimates* the relaxation in the clean (and presumably also in the nearly metallic) region of the phase diagram [26]. To eliminate finite size effects we have increased the size of the system until no changes are observed in our measure. Note that, up to the considered time, $L = 12$ suffices only for $W > 3$, which suggests

that the numerically obtained critical line of Fig. 1 is prone to large finite size effects, at least for the considered interaction strengths. Thus, if that line exists in the $L \rightarrow \infty$ limit, it should move toward higher values of V in the $V - W$ plane.

Although at the MBL transition we expect to observe a steep change in the functional dependence of the correlation functions, the behavior of density fluctuations appear surprisingly smooth over a broad range of parameters. To demonstrate this, we fix W and cross the numerically determined critical line by changing V (see Fig. 1). The correlation function can be reasonably well rescaled by setting $\delta\bar{\rho}(t) \equiv 1 - 4\delta\rho(t)$, while plotting $V^{-0.78}\delta\bar{\rho}(t)$ as a function of rescaled time, $V \cdot t$ (see Fig. 3). The exponent was obtained by fitting. We could not find satisfactory rescaling for fixed V . The initial fast relaxation time may be inferred from Fig. 3, $t_1 \sim 6V^{-1}$. During this time the system dephases across the exact many-body states, which span the initial state. The scaling suggests that, $\delta\rho(t) = \frac{1}{4} - AV^{0.78}f(Vt)$, and therefore assuming its asymptotic validity it should decay to zero at the ergodic-non-ergodic transition $V = V_*$. This yields the form $\delta\rho(V, t \rightarrow \infty) = \frac{1}{4} \left(1 - (V/V_*)^{0.78}\right)$. In particular, the smooth character of the temporal behavior suggests that $V_* > 0.4$. *Thus our numerics suggest that all correlation functions in the region of investigation asymptotically decay to a finite value corresponding to a non-ergodic state.*

To summarize, this work presents, for the first time, a detailed description of the dynamical phase diagram and of how dynamical quantities manifest in the MBL scenario. Although our approach is approximate, it is based on the same approximations that first predicted the existence of MBL [1], and thus should provide important qualitative guidelines to the long-time behavior that is out of reach by more rigorous methods. We find that for all values of interaction and disorder strengths studied, density fluctuations decay in a remarkably slow, non-exponential manner. Furthermore, the dynamics do not qualitatively change in a broad region of parameter space, and are consistent with a non-ergodic phase. This is rather surprising, given that our scan of parameters takes the system across the transition line of Ref. 12 and in the vicinity of the ergodic metal region proposed in Ref. 1. Our results, however, may be viewed as consistent with both works, if the phase boundary of Ref. 12, which based on our finite size analysis is expected to drift upward in the thermodynamic limit, demarcates an “ergodic-non-ergodic” transition where the non-ergodic phase is actually a non-ergodic metal. To resolve these questions would require calculation of the conductivity in addition to the density fluctuations. This is much more difficult to do within the approach described here. Research along these lines will be presented in a future publication.

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